

FRACTIONAL PERIODICITY OF PERSISTENT CURRENTS: A SIGNATURE OF BROKEN INTERNAL SYMMETRY

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We show from the symmetries of the many body Hamiltonian, cast into the form of the Heisenberg (spin) Hamiltonian, that the fractional periodicities of persistent currents are due to the breakdown of internal symmetry and the spin Hamiltonian holds the explanation to this transition. Numerical diagonalizations are performed to show this explicitly. Persistent currents therefore, provide an easy way to experimentally verify broken internal symmetry in electronic systems.

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Remarkable advances in fabrication techniques, now make it possible to confine a few electrons in a conducting wire where electron motion is governed by quantum mechanics, rather than classical mechanics. The system becomes an electron waveguide within the confinement potential. The phase coherence of the electrons is maintained over the sample, making it possible to observe several intrinsic quantum mechanical phenomena including Aharonov-Bohm oscillations, universal conductance fluctuations, quantized conductance in point contact, quenching of Hall resistance in narrow cross [1], current magnification effect [2], etc. A remarkable consequence of such coherence is the existence of equilibrium persistent currents [3] in a ring threaded by an Aharonov-Bohm flux, that was first predicted theoretically [4] and subsequently detected experimentally [5] in mesoscopic systems. Aharonov-Bohm flux here refers to a situation when the magnetic field is restricted to a small region in the center of the ring, and the electrons in the ring do not feel the magnetic field. Although these are equilibrium currents, they can yield information about transport [6] and may help us to understand the effects of electron-electron interaction on transport, using Hamiltonian diagonalization techniques.

Interacting fermions exhibit very novel properties that fascinate scientists for a long time. Interacting nucleons for example has shown many novel features of interactions [7]. Of special relevance to this work, is the discovery that certain heavy nuclei can exhibit rotational excitations, that could not be explained by the shell structure of a spherical nucleus. Initial understanding was provided by Bohr and Mottelson, in terms of collective modes of a deformed nuclei, in the simplest model as rigid rotation of the deformed nucleus. Similar ideas of *internal* symmetry breaking, explained the details of the mass spectra of alkali metal clusters[8], and suggest an existence of static spin-density waves in quantum dots[10]. Indeed, mesoscopic systems give us a unique opportunity to access regimes that do not occur naturally and study a few electrons in man made quantum dots, both experimentally and simultaneously with almost exact theoretical methods. Hence these systems

can give us a rare opportunity to study how few electron properties evolve into macroscopic collective properties as we increase the number of electrons.

Wigner crystalization of electrons is one such bulk phenomenon and is still a very debatable issue, although it was first proposed a very long time ago. We hereby exclude the situation when the quantum mechanical kinetic energy or uncertainty of an electron can be quenched by a strong magnetic field. Theoretically one can find signatures of a crystal structure when one looks at the conditional probability (the probability of finding other electrons when the coordinates of one electron is fixed by hand) of the interacting electrons, while the probability itself (density) does not show any sign of a crystal structure. The conditional probability shows oscillations[9] which suggest broken internal symmetry. However, in finite systems the situation is not so clear due to the fact that the correlation coming from the Pauli exclusion principle alone will cause oscillating conditional probability at short distances, even in noninteracting systems. On the other hand a recent work of Koskinen et al [10] raises the issue that a few electron system in a quantum dot and quantum ring can exhibit broken internal symmetry. Their mean field studies of the electron probability (density) showed a perfect crystal structure. It was subsequently shown [11] that the quantum mechanical superposition of states is destroyed by the non-linearity of the mean field and as a result the internal symmetry is mapped out (as a consequence the angular momentum quantum number does not take integral values anymore). Effects of non-linearity cannot be ignored (the exact cause of non-linearity not being important) and can well lead to a quenching of the quantum mechanical uncertainty and result in Wigner crystals. Hence at this state it would be useful to find some experimental ways of determining if the internal symmetry is broken or not and what are the signatures that one should look for when treating larger systems using approximate methods like mean field theories and effective Hamiltonians. For example, in nuclei, the experimental evidence of such broken symmetry states can be obtained from the rotational spectrum. The purpose of this work is to show that the

measurement of the persistent current can give signature of broken internal symmetry of electronic states in small quantum rings.

The many-body Hamiltonian for electrons in a quasi-1D-ring can be written as

$$H = \sum_i \left(-\frac{\hbar^2}{2m^*} \nabla_i^2 + V(r_i) \right) + \sum_{i < j} \frac{e^2}{4\pi\epsilon_0\epsilon |\vec{r}_i - \vec{r}_j|} \quad (1)$$

where V is the potential confining the electron in the ring. V is assumed to have a circular symmetry. Koskinen *et al* [12, 13] have performed exact numerical computations for a few electrons confined in such a ring and shown that for narrow rings the many-body spectrum can be described essentially exactly with a simple model Hamiltonian

$$H_{eff} = J \sum_i \vec{S}_i \cdot \vec{S}_j + \frac{1}{2I} M^2 + \sum_\alpha \hbar\omega_\alpha n_\alpha \quad (2)$$

where the first term is an antiferromagnetic Heisenberg Hamiltonian, the second term describes rigid rotations of the electron system (M is the centre of mass angular momentum and I is the moment of inertia), and the last term describes the vibrational states of localized electrons. Koskinen *et al* [12, 13] compared the energy spectra of exact diagonalization of Hamiltonian (1) to those of the model Hamiltonian (2) and found an excellent agreement for hundreds of many-body states in rings with from 2 to 7 electrons.

The model Hamiltonian can be understood as a result of localization of electrons and forming a Wigner molecule which is freely rotating in the external potential[12]. Related ideas of electron localization in noncircular dots had been suggested earlier[14, 15]. Assuming localization, the Coulomb energy of the exact Hamiltonian (1) can be expanded around the classical equilibrium positions of electrons. This leads to potential wells at each classical site. The tight binding model of the system can be described by a half filled Hubbard model, which in the limit of the strong Coulomb energy (Hubbard U) leads to the antiferromagnetic Heisenberg model [16]. It is important to note, however, that for our continuous system where the localizing potential is not an external potential, we do not get an insulating phase for the half filled case [17]. The rigid rotation and the vibrations of the localized electrons can be assumed to separate out from the spin Hamiltonian leading to the simple effective Hamiltonian of Eq. (2). The antisymmetry of the total Hamiltonian have to be taken into account by matching the symmetries of the different parts of the wave function (spin, rotations, vibrations)[13]. In the present case when we are studying only the ground state properties (persistent current being a ground state property) the vibrational states do not play any role.

An external magnetic field will bring two additional terms in the model Hamiltonian. The gauge field will change the angular momentum part and the direct interaction with the electron spins will add a Zeeman term.

Since we are interested in the equilibrium persistent currents, we will assume that the magnetic field is confined only inside the ring so that the Zeeman energy is absent. By ignoring the vibrations (which have higher energy than rotations) the model Hamiltonian in the presence of a magnetic field flux ϕ penetrating the ring is

$$H_B = J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j + \frac{(M - N\phi)^2}{2I} \quad (3)$$

where M is the angular momentum, N the number of electrons in the ring and ϕ is the flux through the ring in units of $\phi_0 = hc/e$ i.e., $\phi = \frac{e}{hc} \int \vec{A} \cdot d\vec{r}$ \vec{A} being the vector potential. The strongly interacting case here correspond to $J \rightarrow 0$, $J=0$ being the classical case when the electrons do not overlap. In this case, there is no uncertainty in the internal frame of the system and it is a perfect crystal in its internal frame. It is important to notice that keeping I fixed, the small J limit correspond to a narrow ring with strong correlation and the large J limit approaches the non-interacting case.

The correspondence between (1) and (3) shown in Ref. [12] in the absence of flux, can be easily extended to the case when there is Aharonov-Bohm flux. First of all the Hamiltonian in (3) cannot have any extra contribution from the 2nd term in the Hamiltonian in (1). This is because when we write the Hamiltonian in (1) in terms of a centre of mass coordinate and relative coordinates, the second term contains only relative coordinates, and will only affect the vibrational states, which in turn does not affect the persistent currents. This means that J is independent of flux because the second term in (1) only depends on relative coordinates and is not affected by the flux. Another way to prove this is to show that the Coulomb matrix elements are independent of Aharonov Bohm flux, which can be shown analytically. This is also evident in the numerical calculations [18, 20]. Secondly, the flux also cannot affect the relative motions (kinetic energy part) of the electrons and this was proved in Ref. [21]. The proof essentially puts all the flux dependence on the wavefunction by gauging away the flux dependence of the Hamiltonian. Writing the many body wavefunction in presence of flux as a linear combination of Slater determinants, constructed from the flux dependent, non-interacting, single particle wave functions, it is easy to show that all the flux dependence of the relative coordinates cancel each other. The second term in (3) also directly follow from there, once we put the flux dependence back into the Hamiltonian.

The persistent current can be determined as a derivative of the ground state energy with respect of the flux[3]. Consequently, it is sufficient to study the periodicity of the ground state energy as a function of the flux. First of all it can be shown that the Heisenberg Hamiltonian remains unchanged under the transformation $M \rightarrow M + N$ and so we need to consider only the first N eigen-energies of the system. In Fig. 1 we show a contour plot of the eigen-energies for $N= 4, 5, 6$ and 8 in the $J - \phi$ -plane.

When $J \rightarrow 0$ then the periodicity with flux is ϕ_0/N and correspond to the case when the flux quantum is ϕ_0/N corresponding to the rigid rotor of charge Ne . As J is increased, signifying that the electrons are getting delocalized and overlapping with each other, the periodicity changes smoothly to ϕ_0 . For even number of electrons, ϕ_0/N periodicity first changes over to $\phi_0/2$ periodicity before the full ϕ_0 periodicity is recovered. For odd N also ϕ_0 periodicity changes to $\phi_0/2$ periodicity, which unlike the case of even N , remain all the way up to $J = \infty$. This can also be seen in Fig. 2 where we plot the M values of the ground state for different flux ϕ/ϕ_0 and Jr_0^2 (r_0 being the radius of the ring, $I = Nmr_0^2$). The ground state switches its M values as shown in the figure 2 in the different parameter regimes. While for even N one can see converging phase regions that cannot be extended to infinity, for $N = 5$ the line separating $M = 1$ and $M = 4$ is a vertical line that can be extended to infinity. This is also consistent with the fact that when J is large we should recover the free electron results and odd number of spin-full free electrons in a ring always give $\phi_0/2$ periodicity [19]. But, for even N the ϕ_0/N periodicity first changes to $\phi_0/2$ periodicity as J is increased, and then the free electron result of ϕ_0 periodicity is recovered for very large J .

The value of flux which gives the minimum total energy for large J depends on the number of electrons in the ring. For even particles with $N = 4, 8, 12$, etc. ($N/2$ is even) the minimum is at flux $\phi = \phi_0/2$ (see fig. 3) while for $N = 6, 10$ etc. ($N/2$ is odd) the minimum is at $\phi = 0$. The reason is the symmetry of the solution of the Heisenberg Hamiltonian as can be proved for any N from group theoretical analysis. For odd $N/2$ the minimum energy corresponds to $M = 0$ and the second lowest state has $M = N/2$ while for even $N/2$ the minimum energy has $M = N/2$ and the second lowest state has $M = 0$ (see fig. 3 as an example). In both cases it happens that at a certain region of J , when the angular momentum is increased, the ground state jumps between these two lowest states leading to $\phi_0/2$ periodicity in the total energy and persistent current. When J becomes large enough then the splitting between these two lowest states also become very large and only the ground state of the Heisenberg Hamiltonian matters and ϕ_0 periodicity is obtained. For odd number of electrons (odd N) the situation is different since there are two angular momentum values corresponding to the minimum energy of the Heisenberg Hamiltonian. For noninteracting electrons these two values appear at angular momenta (in the limit of $N \rightarrow \infty$) $N/4$ and $3N/4$. Consequently, there are two equal energy minima leading to $\phi_0/2$ periodicity even at infinitely large values of J . In the case of small number of electrons the energy minimum can not occur exactly at $N/4$ and the ϕ_0 and $\phi_0/2$ periodicities are superimposed as in Fig. 1(b). This signifies that for intermediate J values, when there is no longer any correlation between all the N particles as in a rigid rotor, there still seems to be correlation between electron

pairs leading to quasi-particles with charge $2e$. For odd N since every electron cannot find a pair (similar to the parity effect in superconducting grains), such correlation is not possible. Spin values may or may not change as flux is changed from 0 to ϕ_0 . The sequence of change is depicted in Fig. 2. The ϕ_0/N periodicity occurs when J is small and the splitting between the states is so small that the flux can create transition through all the states.

It should be noted that the flux dependence of the eigenenergies, in a clean ring, should be the same in presence and absence of interactions [21]. A many body eigenenergy, in absence of interactions, should change parabolically with $N\phi$. Our model Hamiltonian in (3) is consistent with this and the flux dependence of a given state is always parabolic in the calculated eigenenergies. However, as the periodicity is reduced by N , the amplitude of the persistent currents is also reduced by N as the Brillouin zone becomes $1/N$ of the non-interacting case. For large J , when we recover the ϕ_0 periodicity, once again the flux dependence of a particular many body state changes parabolically with $N\phi$, all the way up to the non-interacting zone boundary.

The relation of the parameters of the model Hamiltonian (2) to those of the original Hamiltonian (1) require exact diagonalization of the latter. The results of Koskinen et al [12, 13] indicate that the onset of the ϕ_0/N periodicity, which happens at $Jr_0^2 \approx 0.1$, can be obtained with a ring with $V(r) = \frac{1}{2}m^*\omega_0^2(r-r_0)^2$, by choosing (in effective atomic units) $\omega_0 \approx 1/m^*r_0^2$ (for $N = 6$). For a material with $m^* = 0.1$ and $\epsilon = 10$ this condition could be achieved, for example, with $r_0 = 80$ nm and $\omega_0 = 1.7$ meV.

Fractional periodicities of persistent currents in a 1D Hubbard ring has been discussed before [17, 23, 24]. These studies correspond to a situation when there is an externally applied periodic potential or a lattice. In presence of such an externally applied potential the concept of Wigner crystal is not meaningful. The observed fractional periodicities, Kotlyar et al [24] associate with magnon excitations. How this interpretation relates to our findings is an interesting subject of future studies.

Breakdown of internal symmetry of a many body system [10], crystallization of electrons in the bulk (Wigner crystals), fractional periodicities of persistent currents [20] are three different interesting research topics that are brought together in this work. It is shown that fractional periodicity of persistent currents is due to the breakdown of internal symmetry. The Hamiltonian, diagonalized upto 8 electrons in a ring threaded by a flux show this explicitly and symmetry considerations establish this for any N . Broken internal symmetry in electronic systems is of special importance as the interaction between electrons is well known as compared to that between nucleons. It is difficult to observe such broken symmetry states because most of the physical quantities that can be measured, do not depend on whether the internal symmetry is broken or not. In the nuclei, the only evidence of such broken internal symmetry comes from the rotational and

vibrational spectrum of a nuclei. For electrons embedded in a solid the equilibrium persistent currents provide a way to find this evidence. At present a few electron ring can be realized [22] and possibly reveals the much sought experimental proof of broken internal symmetry

in an electronic system.

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Figure Captions

Fig. 1. 2D plot of the energy of the Heisenberg Hamiltonian for electrons in a 1D ring versus Jr^2 and ϕ/ϕ_0 for $N=4$ (Fig. a), 5 (Fig. b), 6 (Fig. c) and 8 (Fig. d). The dark areas are maxima and bright areas are minima. The persistent is the derivative of the energy with respect to the flux and so for the persistent currents dark areas are minima and bright areas are maxima.

Fig. 2. Phase diagram of the ground state angular momentum of the Heisenberg Hamiltonian for electrons in a 1D ring versus Jr^2 and ϕ/ϕ_0 for $N=4$ (Fig. a), 5 (Fig. b), 6 (Fig. c) and 8 (Fig. d). The region with a particular shade denotes the Jr^2 and ϕ/ϕ_0 , corresponding to which the ground state angular momentum is M , where M is designated in the shaded regions as $M(S)$, where S is the total spin.

Fig. 3. States of an 8 electron system in a 1D ring as obtained by diagonalizing the Heisenberg Hamiltonian. $\phi/\phi_0=0$, $Jr^2 = 1.0$, the M values are given at the base and the S values are labeled by the side of each state. The difference between the lowest state and the highest state in the Fig. is $5.651 Jr^2$.

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